Mean field solutions to singlet hopping and superconducting pairing within a two-band Hubbard model

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Abstract

The mean field Green function solution of the two-band singlet-hole Hubbard model for high-T_c superconductivity in cuprates (Plakida, N.M. et al., Phys. Rev. B51, 16599 (1995), JETP 97, 331 (2003)) involves expressions of higher order correlation functions describing respectively the singlet hopping and the superconducting pairing. Rigorous derivation of their values is reported based on the finding that specific invariant classes of polynomial Green functions in terms of the Wannier overlap coefficients ν_{ij} exist.

1 Introduction

The two-band singlet-hole Hubbard model considered by Plakida et al. [1] for the description of the high-T_c superconductivity in cuprates in terms of Hubbard operators (HOs) provides the simplest consistent approach towards the incorporation of the essential features of these systems (strong antiferromagnetic superexchange interaction inside the CuO_2 planes, occurrence of two relatively isolated energy bands around the Fermi level, able to develop $d_{x^2-y^2}$ pairing) such as to describe simultaneously both the normal and the superconducting states within a frame which secures rigorous fulfilment of the basic principles of the quantum mechanics. The equation of motion

method for two-time Green functions [2] was successfully used to derive electron spectra of the model [1] and to incorporate the superconducting state as well [3, 4].

The present paper reports rigorous results for the expressions of two higher order correlation functions which arise in the generalized mean field approximation (GMFA) solution of the Green function (GF) [4]: $\langle X_i^{02} X_j^{20} \rangle$ which describes the *singlet hopping*, and $\langle X_i^{02} N_j \rangle$, which describes the *exchange superconducting pairing interaction*.

The idea proposed in [4] for the evaluation of the average $\langle X_i^{02} N_j \rangle$ can be consistently generalized to yield power series expansions of both statistical averages. We find that the lowest order expressions of the two correlation functions, generically denoted henceforth $\langle X_i^{02} Q_j \rangle$ – where Q_j is either X_j^{20} or N_j, are *obtained in terms of GMFA Green functions.*

This remarkable result follows from the mathematical properties of the Hubbard operators. These allow the definition of characteristic *invariant classes of polynomial Green functions* in terms of the Wannier overlap coefficients ν_{ij}, which are characterized by the property that, under the iteration of the equation of motion, the operator part remains *invariant*, while the polynomial degree in ν_{ij} is increased making thus possible consistent power series expansions in the small parameters ν_{ij}.

2 Statement of the problem

2.1. Hubbard operators. The Hubbard operators (HOs) $X_i^{\alpha\beta} = |i\alpha\rangle\langle i\beta|$ are defined for the four states of the model: $|0\rangle$ (vacuum), $|\sigma\rangle = |\uparrow\rangle$ and $|\bar{\sigma}\rangle = |\downarrow\rangle$ (spin states inside the hole subband; in numerical calculations, $\sigma = \pm 1/2, \bar{\sigma} = -\sigma$), and $|2\rangle = |\uparrow\downarrow\rangle$ (singlet state in the singlet subband).

The multiplication rule holds $X_i^{\alpha\beta} X_i^{\gamma\eta} = \delta_{\beta\gamma} X_i^{\alpha\eta}$. The HOs describing the creation/destruction of single states in a subband are Fermi-like ones and obey the anticommutation relations $\{X_i^{\alpha\beta}, X_j^{\gamma\eta}\} = \delta_{ij}(\delta_{\beta\gamma} X_i^{\alpha\eta} + \delta_{\eta\alpha} X_i^{\gamma\beta})$, while the HOs describing the creation/destruction of singlets, spin and charge densities, particle numbers, are Bose-like ones and obey the commutation relations $[X_i^{\alpha\beta}, X_j^{\gamma\eta}] = \delta_{ij}(\delta_{\beta\gamma} X_i^{\alpha\eta} - \delta_{\eta\alpha} X_i^{\gamma\beta})$. At each lattice site i, the constraint of no double occupancy of any quantum state $|i\alpha\rangle$ is rigorously preserved due to the completeness relation $X_i^{00} + X_i^{\sigma\sigma} + X_i^{\bar{\sigma}\bar{\sigma}} + X_i^{22} = 1$.

The *particle number operator at site* i is given by

$$N_i = X_i^{\sigma\sigma} + X_i^{\bar{\sigma}\bar{\sigma}} + 2X_i^{22}. \tag{1}$$

We define the *Hubbard p-form of labels* $(\alpha\beta, \gamma\eta)$,

$$\tau_{p,i}^{\alpha\beta,\gamma\eta} = \sum_{j\neq i} \nu_{ij}^{p} X_i^{\alpha\beta} X_j^{\gamma\eta}, \quad p = 1, 2, \cdots, \tag{2}$$

where the meanings of HOs $X_i^{\alpha\beta}$ and $X_j^{\gamma\eta}$ depend on the context. The Wannier overlap coefficients ν_{ij} are small quantities rapidly decreasing with the intersite distance $r_{ij} = |\mathbf{r}_j - \mathbf{r}_i|$ (see, e.g., [5, 6] and references quoted therein). The nearest neighbour values $\nu_{i,i\pm a_{x/y}} = \nu_1 \simeq -0.14$ and next nearest ones $\nu_{i,i\pm a_x \pm a_y} = \nu_2 \simeq -0.02$ considered in [1] are typical.

2.2. Model Hamiltonian. The Hamiltonian of the model [1] can be rewritten in terms of linear Hubbard forms describing hopping processes as follows

$$\begin{aligned} H = E_1 \sum_{i,\sigma} X_i^{\sigma\sigma} + E_2 \sum_{i} X_i^{22} + \\ + \mathcal{K}_{11} \sum_{i,\sigma} \tau_{1,i}^{\sigma 0,0\sigma} + \mathcal{K}_{22} \sum_{i,\sigma} \tau_{1,i}^{2\sigma,\sigma 2} + \mathcal{K}_{12} \sum_{i,\sigma} 2\sigma (\tau_{1,i}^{2\bar{\sigma},0\sigma} + \tau_{1,i}^{\sigma 0,\bar{\sigma}2}), \end{aligned} \tag{3}$$

where the summation label i runs over the sites of an infinite two-dimensional square array the lattice constants of which, $a_x = a_y$, are defined by the underlying single crystal structure.

In Eq. (3), $E_1 = \tilde{\varepsilon_d} - \mu$ and $E_2 = 2E_1 + U_{eff}$, where $\tilde{\varepsilon_d}$ is the renormalized energy of a d-hole, μ is the chemical potential, while $U_{eff} \equiv \Delta \approx \Delta_{pd} = \varepsilon_p - \varepsilon_d$ is an effective Coulomb energy corresponding to the difference between the hole energy levels for oxygen and copper.

Keeping in mind that the lower label 1 refers to one-hole states, while the lower label 2 to singlet states, the quantities $\mathcal{K}_{ab} = 2t_{pd}K_{ab}$ are characteristic hopping energies for either inband ($a = b$) or interband ($a \neq b; \mathcal{K}_{12} = \mathcal{K}_{21}$) transitions between the two bands of the model. Here t_{pd} denotes the hopping p-d integral and K_{ab} are numerical coefficients coming from hybridization effects between the holes and the singlets [1].

The translational invariance of the system gives

$$(\tau_i^{\alpha\beta,\gamma\eta})^\dagger = -\tau_i^{\beta\alpha,\eta\gamma} = \tau_i^{\eta\gamma,\beta\alpha}, \tag{4}$$

which secures the hermiticity of the model Hamiltonian H.

2.3. Mean field approximation. The quasi-particle spectrum and superconducting pairing within the model Hamiltonian (3) are obtained [3, 4]

from the two-time 4×4 matrix Green function (GF) in Zubarev notation [2]

$$\tilde{G}_{ij\sigma}(t-t') = \langle\langle \hat{X}_{i\sigma}(t) \,|\, \hat{X}^{\dagger}_{j\sigma}(t')\rangle\rangle = -i\theta(t-t')\langle\{\hat{X}_{i\sigma}(t), \hat{X}^{\dagger}_{j\sigma}\}\rangle. \tag{5}$$

where $\langle\cdots\rangle$ denotes the statistical average over the Gibbs grand canonical ensemble.

The GF (5) is defined for the four-component Nambu column operator

$$\hat{X}_{i\sigma} = (X_i^{\sigma 2}\ X_i^{0\bar{\sigma}}\ X_i^{2\bar{\sigma}}\ X_i^{\sigma 0})^{(\mathrm{T})} \tag{6}$$

The operator $\hat{X}^{\dagger}_{j\sigma} = (X_j^{2\sigma}\ X_j^{\bar{\sigma}0}\ X_j^{\bar{\sigma}2}\ X_j^{0\sigma})$ is the adjoint of $\hat{X}_{j\sigma}$. In (6), the superscript (T) denotes the transposition. Here and in what follows, due to translational invariance, the notation $\mathcal{G}_{ij}$ points to the dependence of the quantity $\mathcal{G}$ of interest on the *distance* $r_{ij} = |\mathbf{r}_j - \mathbf{r}_i|$ between the position vectors of the lattice sites j and i respectively.

The derivation of the GF within GMFA needs the knowledge of the *frequency matrix*,

$$\tilde{\mathcal{A}}_{ij\sigma} = \langle\{[\hat{X}_{i\sigma}, H], \hat{X}^{\dagger}_{j\sigma}\}\rangle. \tag{7}$$

Direct calculations [4] show that the *normal* matrix elements of $\tilde{\mathcal{A}}_{ij\sigma}$ contain *one-site* ($i=j$) GMFA hopping correlation function which result in $\mathcal{O}(\mathcal{K}_{ab}\nu_{ij})$ renormalizations of the energy parameters E_1 and E_2, as well as *two-site* ($i\neq j$) hopping generated *higher order* correlation functions bringing two distinct kinds of contributions to $\tilde{\mathcal{A}}_{ij\sigma}$: *charge-spin* correlations (which can be conveniently subdivided into *charge-charge*, $\langle N_i N_j\rangle$, and *spin-spin*, $\langle \mathbf{S}_i\mathbf{S}_j\rangle = \langle X_i^{\sigma\bar{\sigma}} X_j^{\bar{\sigma}\sigma}\rangle$, correlations) and the *singlet hopping* correlation function $\langle X_i^{02} X_j^{20}\rangle$ (singlet destruction at site i followed by singlet creation at site j).

There are three distinct matrix elements out of the eight normal matrix elements of $\tilde{\mathcal{A}}_{ij\sigma}$ containing $\langle X_i^{02} X_j^{20}\rangle$:

$$(\sigma 2, 2\sigma) \qquad -\mathcal{K}_{11}\nu_{ij}\langle X_i^{02} X_j^{20}\rangle \tag{8}$$

$$(0\bar{\sigma}, \bar{\sigma}0) \qquad -\mathcal{K}_{22}\nu_{ij}\langle X_i^{02} X_j^{20}\rangle \tag{9}$$

$$(\sigma 2, \bar{\sigma}0) \qquad -2\sigma\cdot\mathcal{K}_{21}\nu_{ij}\langle X_i^{02} X_j^{20}\rangle \tag{10}$$

The only non-vanishing *anomalous* matrix elements of $\tilde{\mathcal{A}}_{ij\sigma}$ are [4] the hopping generated *two-site* contributions involving the higher order correlation function $\langle X_i^{02} N_j\rangle$. This provides the *exchange superconducting pairing mechanism* originating in the interaction of an anomalous pair of particles at

a same site i but in different subbands ($X_i^{02} = X_i^{0\sigma} X_i^{\sigma 2}$), with the surrounding particle distribution at the neighbouring site j described by the particle number operator N_j, Eq. (1). The structure of the anomalous part of $\tilde{\mathcal{A}}_{ij\sigma}$ is very special:

$$\begin{array}{lll} (\sigma 2, \bar{\sigma} 2) & 2\bar{\sigma}\cdot\mathcal{K}_{21}\nu_{ij}\langle X_i^{02} N_j\rangle & (11) \\ (0\bar{\sigma}, \sigma 0) & 2\sigma\cdot\mathcal{K}_{21}\nu_{ij}\langle X_i^{02} N_j\rangle & (12) \\ (\sigma 2, 0\sigma) & \frac{1}{2}(\mathcal{K}_{11}+\mathcal{K}_{22})\nu_{ij}\langle X_i^{02} N_j\rangle & (13) \\ (0\bar{\sigma}, \bar{\sigma} 2) & -\frac{1}{2}(\mathcal{K}_{11}+\mathcal{K}_{22})\nu_{ij}\langle X_i^{02} N_j\rangle & (14) \end{array}$$

The other anomalous matrix elements are obtained by complex conjugation.

3 Fundamental relationships

From the spectral theorem [2],

$$\langle X_i^{02} Q_j\rangle = \frac{i}{2\pi}\int_{-\infty}^{+\infty} \frac{\mathrm{d}\omega}{1-\mathrm{e}^{-\beta\omega}} \Big[\langle\langle X_i^{02}|Q_j\rangle\rangle_{\omega+i\varepsilon} - \langle\langle X_i^{02}|Q_j\rangle\rangle_{\omega-i\varepsilon}\Big], \qquad (15)$$

where the labels $\pm i\varepsilon$, $\varepsilon = 0^+$, refer to the retarded/advanced Green functions respectively. Since both X_i^{02} and Q_j are bosonic Hubbard operators, the thermodynamic factor in the denominator is $1-\mathrm{e}^{-\beta\omega}$ and the two Green functions are defined in terms of the commutators of the two operators, i.e.,

$$\langle\langle X_i^{02}(t)|Q_j(t')\rangle\rangle = -i\theta(t-t')\langle[X_i^{02}(t), Q_j(t')]\rangle \qquad (16)$$

for the retarded Green function and a similar definition for the advanced one.

By differentiation with respect to t and use of Fourier transform, we get the following basic result for the two Green functions in the $(\mathbf{r},\omega)$-representation required by Eq. (15) (for the sake of simplicity, $\pm i\varepsilon$ terms are omitted):

$$\begin{aligned}(\omega - E_2)\langle\langle X_i^{02}|Q_j\rangle\rangle_\omega =& -\mathcal{K}_{11}\sum_\sigma \langle\langle \tau_{1,i}^{\sigma 2,0\sigma}|Q_j\rangle\rangle_\omega + \mathcal{K}_{22}\sum_\sigma \langle\langle \tau_{1,i}^{0\sigma,\sigma 2}|Q_j\rangle\rangle_\omega + \\ & + \mathcal{K}_{21}\sum_\sigma 2\sigma\Big(\langle\langle \tau_{1,i}^{0\bar{\sigma},0\sigma}|Q_j\rangle\rangle_\omega - \langle\langle \tau_{1,i}^{\sigma 2,\bar{\sigma}2}|Q_j\rangle\rangle_\omega\Big) \qquad (17)\end{aligned}$$

Theorem 1 *Let* $g_{2p-1}^{\alpha\beta,\gamma\eta} \equiv \langle\langle \tau_{2p-1,i}^{\alpha\beta,\gamma\eta} | Q_j \rangle\rangle_\omega$ *be a generic notation of the* extensions to Hubbard $(2p-1)$-forms *(2) of the four Green functions which enter the r.h.s. of Eq. (17). Then the recurrence relations hold,*

$$g_{2p-1}^{\sigma 2,0\sigma} = \frac{\nu_{ij}^{2p-1} M'_{ij\sigma}}{\omega - E_2} - \frac{\mathcal{K}_{22}\nu_{ij}^{2p} P''_{ij\sigma}}{(\omega - E_2)^2} + \frac{\mathcal{K}_{11}^2 + \mathcal{K}_{22}^2}{(\omega - E_2)^2} g_{2p+1}^{\sigma 2,0\sigma} - \frac{2\mathcal{K}_{11}\mathcal{K}_{22}}{(\omega - E_2)^2} g_{2p+1}^{0\sigma,\sigma 2} \tag{18}$$

$$g_{2p-1}^{0\sigma,\sigma 2} = \frac{\nu_{ij}^{2p-1} M''_{ij\sigma}}{\omega - E_2} + \frac{\mathcal{K}_{11}\nu_{ij}^{2p} P''_{ij\sigma}}{(\omega - E_2)^2} - \frac{2\mathcal{K}_{11}\mathcal{K}_{22}}{(\omega - E_2)^2} g_{2p+1}^{\sigma 2,0\sigma} + \frac{\mathcal{K}_{11}^2 + \mathcal{K}_{22}^2}{(\omega - E_2)^2} g_{2p+1}^{0\sigma,\sigma 2} \tag{19}$$

$$g_{2p-1}^{0\bar\sigma,0\sigma} = \frac{\nu_{ij}^{2p-1} M'''_{ij\sigma}}{\omega - 2E_1} + \frac{2\sigma\mathcal{K}_{21}\nu_{ij}^{2p} (P'''_{ij\sigma} + P^{IV}_{ij\sigma})}{(\omega - 2E_1)(\omega - E_2)} + \frac{(2\mathcal{K}_{21}\cdot 2\sigma)^2}{(\omega - 2E_1)(\omega - E_2)} g_{2p+1}^{0\bar\sigma,0\sigma} \tag{20}$$

$$g_{2p-1}^{\sigma 2,\bar\sigma 2} = \frac{\nu_{ij}^{2p-1} M^{IV}_{ij\sigma}}{\omega - (E_2 + \Delta)} + \frac{2\bar\sigma\mathcal{K}_{21}\nu_{ij}^{2p} (P^{V}_{ij\sigma} + P^{VI}_{ij\sigma})}{[\omega - (E_2 + \Delta)](\omega - E_2)} + \frac{(2\mathcal{K}_{21}\cdot 2\bar\sigma)^2}{[\omega - (E_2 + \Delta)](\omega - E_2)} g_{2p+1}^{\sigma 2,\bar\sigma 2} \tag{21}$$

where the coefficients $M_{ij\sigma}$ *and* $P_{ij\sigma}$*, given in Table 1, are statistical averages following from equal time commutator terms.*

The proof is immediate if we write the equations of motion of the Green functions mentioned in the l.h.s. and iterate once.

Table 1: Equal time commutators arising in the recurrence relations (18)–(21) as coefficients of ν_{ij}^{2p-1} and ν_{ij}^{2p}

ν_{ij}^{2p-1}	$Q_j = X_j^{20}$	$Q_j = N_j$	ν_{ij}^{2p}	$Q_j = X_j^{20}$	$Q_j = N_j$
$M'_{ij\sigma}$	$-\langle X_i^{\sigma 2} X_j^{2\sigma}\rangle$	$\langle X_i^{\sigma 2} X_j^{0\sigma}\rangle$	$P'_{ij\sigma}$	0	0
$M''_{ij\sigma}$	$\langle X_i^{0\sigma} X_j^{\sigma 0}\rangle$	$\langle X_i^{0\sigma} X_j^{\sigma 2}\rangle$	$P''_{ij\sigma}$	$\langle X_i^{\sigma\sigma}(X_j^{00} - X_j^{22})\rangle$	$\langle X_i^{\sigma\sigma} X_j^{02}\rangle$
$M'''_{ij\sigma}$	$-\langle X_i^{0\bar\sigma} X_j^{2\sigma}\rangle$	$\langle X_i^{0\bar\sigma} X_j^{0\sigma}\rangle$	$P'''_{ij\sigma}$	$-\langle X_i^{02} X_j^{20}\rangle$	0
$M^{IV}_{ij\sigma}$	$\langle X_i^{\sigma 2} X_j^{\bar\sigma 0}\rangle$	$\langle X_i^{\sigma 2} X_j^{\bar\sigma 2}\rangle$	$P^{IV}_{ij\sigma}$	$\langle X_i^{00}(X_j^{00} - X_j^{22})\rangle$	$2\langle X_i^{00} X_j^{02}\rangle$
			$P^{V}_{ij\sigma}$	$\langle X_i^{02} X_j^{20}\rangle$	0
			$P^{VI}_{ij\sigma}$	$\langle X_i^{22}(X_j^{00} - X_j^{22})\rangle$	$2\langle X_i^{22} X_j^{02}\rangle$

The *p-form class invariance* of the abovementioned Green functions is a straightforward consequence of the commutation and multiplication rules

satisfied by the Hubbard operators. It allows the derivation of the statistical averages $\langle X_i^{02} X_j^{20} \rangle$ and $\langle X_i^{02} N_j \rangle$ as power series of the small parameters of the model $\mathcal{K}_{11}\nu_{ij}$, $\mathcal{K}_{22}\nu_{ij}$, and $\mathcal{K}_{21}\nu_{ij}$.

While the coefficients of the odd powers of the series expansions are obtained in terms of GMFA Green functions, those of the even powers are still defined in terms of Green functions beyond GMFA. From the point of view of the practical implications, it is an academic question whether it would be possible to express them in terms of GMFA Green functions as well. The lowest order approximations provide the most important contributions to the observables. The question is whether the corresponding statistical averages quoted in the Table 1 are really significant or not. This point is discussed in the next section.

4 Significant lowest order terms

The results derived in the previous section show that the statistical averages $\langle X_i^{02} Q_j \rangle$ are obtained as power series of ν_{ij}, with the contributions coming from the poles of the Green functions given by integrals of the form

$$I_{mn}(\omega_1, \omega_2) \;=\; I_{mn}^{-}(\omega_1, \omega_2) - I_{mn}^{+}(\omega_1, \omega_2), \quad m+n \geq 2, \quad m, n > 0, \tag{22}$$

$$I_{mn}^{\mp}(\omega_1, \omega_2) \;=\; \frac{i}{2\pi} \int_{-\infty}^{+\infty} \frac{\mathrm{d}\omega}{1 - \mathrm{e}^{-\beta\omega}} \frac{1}{[\omega - (\omega_1 \mp i\varepsilon)]^m} \cdot \frac{1}{[\omega - (\omega_2 \mp i\varepsilon)]^n} \tag{23}$$

The calculation of these integrals is standard: they are extended in corresponding complex half-planes $z = (\omega, \Im z \lessgtr 0)$, with half-circles at the three existing poles: $z = 0$, $z = \omega_1 \pm i\varepsilon$, $z = \omega_2 \pm i\varepsilon$. The obtained contour integrals are calculated in two alternatives ways: using the residue theorem, and estimating them along the pieces of the involved contours.

Retaining the lowest order contributions to $\langle X_i^{02} Q_j \rangle$ only, we get:

$$\begin{aligned}
\langle X_i^{02} Q_j \rangle &= I_{20}(E_2) c_1^{\sigma 2, 0\sigma} + I_{11}(E_2, 2E_1) c_1^{0\bar{\sigma}, 0\sigma} + I_{11}(E_2 + \Delta, E_2) c_1^{\sigma 2, \bar{\sigma} 2} + \mathcal{O}(\nu_{ij}^2), \\
c_1^{\sigma 2, 0\sigma} &= -(2\mathcal{K}_{11}\nu_{ij}) M'_{ij\sigma} + (2\mathcal{K}_{22}\nu_{ij}) M''_{ij\sigma}, \\
c_1^{0\bar{\sigma}, 0\sigma} &= 2\sigma (2\mathcal{K}_{21}\nu_{ij}) M'''_{ij\sigma}, \\
c_1^{\sigma 2, \bar{\sigma} 2} &= 2\bar{\sigma} (2\mathcal{K}_{21}\nu_{ij}) M^{IV}_{ij\sigma}, \\
I_{20}(E_2) &= \frac{1}{\beta E_2^2} - \frac{\beta \mathrm{e}^{-\beta E_2}}{(1 - \mathrm{e}^{-\beta E_2})^2}
\end{aligned}$$

$$I_{11}(E_2{,}2E_1){=}\frac{1}{2\beta E_1E_2}-\frac{1}{\Delta}\cdot\frac{1}{1-\mathrm{e}^{-2\beta E_1}}+\frac{1}{\Delta}\cdot\frac{1}{1-\mathrm{e}^{-\beta E_2}}$$
$$I_{11}(E_2{+}\Delta{,}E_2){=}\frac{1}{\beta E_2(E_2{+}\Delta)}+\frac{1}{\Delta}\cdot\frac{1}{1-\mathrm{e}^{-\beta(E_2+\Delta)}}-\frac{1}{\Delta}\cdot\frac{1}{1-\mathrm{e}^{-\beta E_2}}. \tag{24}$$

Theorem 2 *The lowest order power series expansions of the correlation functions $\langle X_i^{02}X_j^{20}\rangle$ and $\langle X_i^{02}N_j\rangle$ are obtained in terms of GMFA correlation functions as follows:*

For hole-doped *systems:*

$$\langle X_i^{02}X_j^{20}\rangle \simeq 2\bar{\sigma}\frac{\mathcal{K}_{21}\nu_{ij}}{\Delta}\langle X_i^{\sigma 2}X_j^{\bar{\sigma}0}\rangle; \quad \langle X_i^{02}N_j\rangle \simeq 2\bar{\sigma}\frac{\mathcal{K}_{21}\nu_{ij}}{\Delta}\langle X_i^{\sigma 2}X_j^{\bar{\sigma}2}\rangle. \tag{25}$$

For electron-doped *systems:*

$$\langle X_i^{02}X_j^{20}\rangle \simeq 2\bar{\sigma}\frac{\mathcal{K}_{21}\nu_{ij}}{\Delta}\langle X_i^{0\bar{\sigma}}X_j^{2\sigma}\rangle; \quad \langle X_i^{02}N_j\rangle \simeq 2\sigma\frac{\mathcal{K}_{21}\nu_{ij}}{\Delta}\langle X_i^{0\bar{\sigma}}X_j^{0\sigma}\rangle. \tag{26}$$

Indeed, for hole-doped systems, the Fermi level lays in the upper *singlet subband*, such that we get the energy parameter estimates $E_1 \simeq E_2 \simeq -\Delta$. This yields $I_{20}(E_2) \simeq I_{11}(E_2, 2E_1) \simeq 0$, while $I_{11}(E_2 + \Delta, E_2) \simeq (2\Delta)^{-1}$, therefrom Eqs. (25) follow.

For electron-doped systems, the Fermi level lays in the upper *hole subband*, and this yields the energy parameter estimates $E_1 \simeq 0,\ E_2 \simeq \Delta$. This results in $I_{20}(E_2) \simeq I_{11}(E_2 + \Delta, E_2) \simeq 0$, while $I_{11}(E_2, 2E_1) \simeq (2\Delta)^{-1}$, hence Eqs. (26) follow.

5 Discussion of the results

Corroboration of Eqs. (8) to (14) with the results stated in Theorem 2 show that, both in hole-doped and electron-doped cuprates, the dominant contributions to the singlet hopping and the exchange superconducting pairing are second order effects described by GMFA correlation functions. In (25) and (26) there occurs a *same* small parameter, $\mathcal{K}_{21}\nu_{ij}/\Delta$, for the description of all the involved higher order correlation functions with, however, *specific* GMFA correlation functions. Thus, the singlet hopping proceeds by $i \rightleftarrows j$ jumps of a particle from the upper energy subband to the lower energy subband. The anomalous superconducting pairing involves two spin states at

neighbouring lattice sites i and j, both with energies in that subband which crosses the Fermi level. However, while both processes are given by small $\mathcal{O}(\nu_{ij}^2)$ quantities, their consequences are quite different.

The non-vanishing singlet hopping brings a small correction to the energy terms entering the normal part of $\tilde{\mathcal{A}}_{ij\sigma}$. Therefore, the decoupling ansatz $\langle X_i^{02} X_j^{20}\rangle \approx \langle X_i^{02}\rangle\langle X_j^{20}\rangle = 0$ used in [1] does not substantially modify the general picture obtained for the normal state.

On the other side, the derivation of the correct GMFA contribution to $\langle X_i^{02} N_j\rangle$ is essential for understanding the pairing mechanism emerging within the model. Under the assumption of uniform hopping, $K_{11} = K_{22} = K_{21} = K$, Eqs. (11)–(14) and (25)–(26) result in the well-known AFM exchange interaction energy of the t-J model, $J = 4t^2/\Delta$, for spins on nearest neighbour sites and an effective hopping parameter $t = t_{pd} K \nu_1$.

In fact, the occurrence of different hopping coefficients in Eqs. (8)–(14) (ref. [1], reported the values $K_{22} \simeq -0.477$, $K_{11} \simeq -0.887$, $K_{12} = K_{21} \simeq 0.834$) points to the existence of three *asymmetric* processes depending on the initial and the final energy subbands connected by the higher order correlation functions $\langle X_i^{02} X_j^{20}\rangle$ or $\langle X_i^{02} N_j\rangle$ respectively.

Finally, the present analysis strengthens the discussion in [4] concerning the unreliability of the approach of reference [7] towards the derivation of a GMFA expression for $\langle X_i^{02} N_j\rangle$ based on the use of the Roth decoupling procedure which uncouples the Hubbard operators at a same site,

$$\langle X_i^{02} N_j\rangle = \langle X_i^{0\sigma} X_i^{\sigma 2} N_j\rangle = \langle c_{i\sigma} c_{i\bar{\sigma}} N_j\rangle \rightarrow \langle\langle c_{i\sigma}(t) | c_{i\bar{\sigma}}(t') N_j(t')\rangle\rangle.$$

Therefore, the consequences following from this decoupling, namely that special interstitial excitations ("cexons") should appear and play an important role in the occurrence of superconductivity in cuprates, are artifacts of the procedure without actual physical meaning.

6 Conclusions

We reported a method for evaluating two higher order correlation functions describing respectively the singlet hopping and the superconductivity pairing within the two-time Green function approach to the solution of the two-band singlet-hole Hubbard model (3) considered by Plakida et al. [1, 4] for the description of the physical properties of the high-T_c superconductivity in cuprates. Both in hole-doped and electron-doped cuprates, the dominant

contributions to the two processes are found to be second order effects described by GMFA correlation functions.

The derived results are rigorously established. For the two discussed processes, they rest on the occurrence of specific *invariant* classes of Green functions with respect to the operators of the Hubbard 1-forms entering the equation of motion (17), allowing therefrom powers series expansions in terms of the small Wannier overlap coefficients ν_{ij}.

The singularity coming at the Fermi level from the thermodynamic factor $(1-e^{-\beta\omega})^{-1}$ is canceled by a corresponding singularity coming from the pole of the Green function at the Fermi level. From the point of view of the properties of the functions of complex variables, at $\omega = 0$ there arises a pole of the second order yielding the finite second order contributions found in the previous section.

We have to remark that the existence of a non-vanishing commutator $[X_i^{02}, H]$ is essential. Since $[N_i, H] = [X_i^{\sigma\bar{\sigma}}, H] = 0$, the method described in this paper cannot be used to the GMFA evaluation of the charge-charge and spin-spin correlation functions.

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